

## Separation of cross-relaxation and exchange in two-site spin systems without resolved couplings

Klochkov V., Karatayeva F., Shaikhutdinov R., Khairutdinov B., Molins M., Pons M.  
*Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia*

---

### Abstract

Variable temperature two-dimensional nuclear Overhauser enhancement experiment (2-D NOESY) is used to extract the rate constants and cross-relaxation rates that contribute to the same cross-peaks in NOESY spectra. Rate constants ( $k_{AB}$ ) and cross-relaxation rates ( $R_{AB}$ ) for two-site spin systems are related to the ratio between the cross-peak and diagonal peak integrals ( $F$ ) by the expression:  $R_{AB} - k_{AB} = (1/2 \tau_m) \ln[(1 - F)/(1 + F)]$ , where  $\tau_m$  is the mixing time. As a model, we investigated the exchange processes in a system of dimer calix[4]arenes of  $C_{4v}$  symmetrical configuration with guest inclusion (benzene or benzene- $d_6$ ), where the measurement of exchange processes is hindered by the presence of strong nuclear Overhauser enhancement between protons in adjacent aromatic rings in the cone conformation of the calix[4]arene.

---